

CLAIMS:

1. A method of optimizing parameter values in a process of producing a product, said process being essentially controlled by a set of n parameters X_i affecting a set of k properties Y_j characterizing the product, said method comprising the steps of:

- i) assigning values to a set of k property weights w_j representing relative importance of said properties Y_j for the characterization of said product;
- ii) establishing property behavior mathematical relations giving an estimated property Ye_j for each said property Y_j in terms of said parameters X_i from given parameter data and associated property data;
- iii) using said property weights w_j to establish a goal function in terms of property weighted deviations between the estimated properties Ye_j and corresponding specified goal values for said properties Y_j ; and
- iv) minimizing the goal function to generate a set of n optimal parameter values for said parameters X_i .

2. A method according to claim 1, wherein said product is a composition, said set of optimal parameter values characterizing an optimal formulation for the composition.

3. A method according to claim 1, wherein said product is a pharmaceutical product, said set of optimal parameter values characterizing an optimal formulation for the pharmaceutical product.

4. A method according to claim 1, 2 or 3, wherein the values for said property weights w_j are obtained using an algorithm based on an analytic hierarchy process.

5. A method according to claim 4, wherein said given property data are obtained through a number l of experimental runs of said process using said given parameter data, each said run using a distinct set of values for said given parameter data.

6. A method according to claim 5, wherein $l \geq n+1$.

7. A method according to any one of claims 1 to 6, wherein said goal function is expressed as follows:

$$G(X_1, \dots, X_n) = \sum_{j=1}^k w_j^2 (Y_{e_j} - O_j)^2$$

wherein O_j are said specified goal values for said properties Y_j . A method according to claim 7, wherein said minimizing step is performed by successive iterations of:

$$G(X_1, \dots, X_n) = \sum_{i=1}^k [f_i(X_1, \dots, X_n)]^p.$$

8. A method according to claim 7, wherein said goal function is minimized according to one or more specified ranges (a_i, b_i) wherein $a_i < X_i < b_i$ for one or more of said optimal parameter values.

9. A method according to any one of claims 1 to 8, further comprising the steps of:

- i) performing experimentally said process using said set of optimal parameters values to obtain corresponding experimental values for said properties Y_j ,
- ii) ranking said set of optimal parameters values over predetermined alternative sets of parameters values for said X_i .

10. A method according to claim 9, wherein said ranking step is performed using an algorithm based on an analytic hierarchy process.

11. A method according to claim 9 or 10, further including the step of:

- i) incorporating said set of optimal parameters values and said corresponding experimental values for said properties Y_j respectively into said given parameter and associated property data;
- ii) repeating said steps ii) to iv) to generate a new set of optimal parameters values for said parameters X_i .

12. A method according to any one of claims 1 to 11, wherein said product is a pharmaceutical product.

13. A method according to any one of claims 1 to 11, wherein said product is a product.

14. A method according to claim 13, wherein said step of calculating comprises:

- i) establishing property behavior mathematical relations giving an estimated property Ye_j for each said property Y_j in terms of said parameters X_i from said parameter data and associated property data;
- ii) using said property weights w_j to establish a process goal function in terms of property weighted deviations between the estimated properties Ye_j and corresponding specified goal values for said properties Y_j ; and
- iii) minimizing the process goal function to generate a set of optimal parameter values for said parameters X_i .

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15. A method according to claim 14, wherein the values for said property weights w_j are obtained by an algorithm based on an analytic hierarchy process.

16. A method according to claim 13, 14 or 15, wherein $l = n + 1$.

17. A method according to any one of claims 14 to 16, wherein said goal function is expressed as follows:

$$G(X_1, \dots, X_n) = \sum_{j=1}^k w_j^2 (Y_{e_j} - O_j)^2$$

wherein O_j are said specified goal values for said properties Y_j .

18. A method according to claim 17, wherein said minimizing step is performed through successive iterations.

19. A method according to claim 18, wherein said goal function is minimized according to one or more specified ranges (a_i, b_i) wherein $a_i < X_i < b_i$ for one or more of said optimal parameters values.

20. A method according to claim 14, further comprising the steps of:
performing experimentally said process using said set of optimal parameters values to obtain corresponding experimental values for said properties Y_j ;

ranking said set of optimal parameters values over predetermined alternative sets of parameters values for said X_i .

21. A method according to claim 20, wherein said ranking step is performed through an algorithm based on an analytic hierarchy process.

22. A method according to claim 21, further including the steps of: incorporating said set of optimal parameters values and said corresponding experimental values for said properties Y_j respectively into said given parameter and associated property data, repeating said steps a), b) and d) to generate a new set of optimal parameters values for said parameters X_i .

23. A method according to any one of claims 13 to 22, wherein said product is a pharmaceutical product.

24. A computer program product performing the method according to any one of claims 1 to 23.

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